SIMULATION STUDY AND PERFORMANCE ANALYSIS OF $FAPbI_3$ BASED HETEROJUNCTION SOLAR CELL USING SCAPS-1D TOOL

SHORT SYNOPSIS

Submitted in partial fulfillment of the requirement of the degree of

DOCTOR OF PHILOSOPHY

by

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DECLARATION BY THE SCHOLAR

I hereby declare that the short synopsis entitled "**Simulation Study and Performance Analysis of $FAPbI_3$ based heterojunction Solar cell using SCAPS-1D Tool**" being submitted in partial fulfillment of the requirement for the degree of Doctor of Philosophy in the Department of Science (Physics) under the School of Sciences of Manav Rachna University, Faridabad during the academic year 2024-25.

It is the work that is expected to be carried out under the supervision of **Dr. Anshuman Sahai** and co- supervision of **Dr. Shiv Kumar Dixit.**

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CERTIFICATE BY SUPERVISOR(S)

This is to certify that, the short synopsis entitled "**Simulation Study and Performance Analysis of $FAPbI_3$ based heterojunction Solar cell using SCAPS-1D Tool**" is an original piece of work done by research scholar Yogmaya Sharma under the supervision of Dr. Anshuman Sahai and co- supervision of Dr. Shiv Kumar Dixit for the degree of Doctor of Philosophy in the Department of Sciences (Physics) under the School of Sciences of Manav Rachna University, Faridabad during the academic year 2024-25.

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ABSTRACT

Lead halide perovskites solar cells have gained immense popularity due to their low cost and high-power conversion efficiency (PCE) as reported ~ 25% till date [1]. But limited absorption, hysteresis and device stability of perovskites solar cells are some issues that need to be resolved. We have analyzed the formamidinium lead tri-iodide ($FAPbI_3$) based solar cell. It has been investigated how adding a NiOx hole transport layer affects the solar cell's power conversion efficiency. Without NiO layer devices, they show very low efficiency of 6.06% and J_{sc} of 23.02 mA/cm^2. However, HTL is very important in device structure, and we observed 22.27 % of PCE and 25.67 mA/cm^2 of J_{sc} after incorporation of NiO layer. Using the SCAPS-1D software tool, the impact of thickness, doping density, total defect density, and the width of the electron transport layer (ETL) and hole transport layer (HTL) on the PCE has been examined. After optimization of process parameters $FAPbI_3$ can replace other already existing lead-based structures and may be commercialized.

Using C-60 and SnO_2 (tin oxide) as the ETL layer, we have investigated the $FAPbI_3$ in detail in this work. Due to its fast electron mobility, high optical transmittance, low temperature processing capability, and appropriate energy level alignment with perovskite absorber, tin oxide has emerged as a particularly interesting candidate material.

Keywords: Perovskite solar cell, Electron Trasport Layer, Power conversion efficiency, Hole Transport layer, Doping.

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1. Introduction

Solar energy is the cleanest and most abundant energy resource present on earth. The energy which is liberated out by the sun reaches the earth in small pieces. These are known as photons. Energy is released when the photon strikes the atom. With the help of photovoltaic effect (generating current or voltage in a material by absorbing light energy) electric energy is produced by converting light energy using solar cell. (Fig-1).

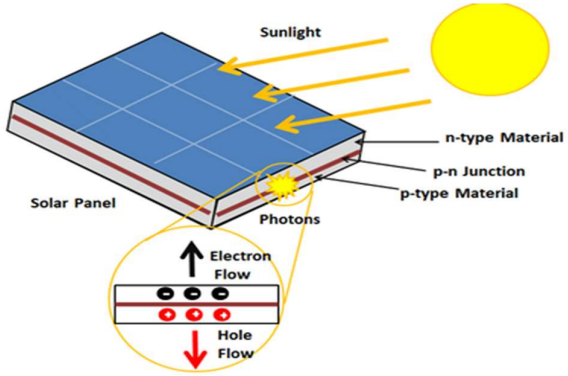

Fig.-1. Typical Solar Cell

The research on solar cells represents a central project at the forefront of sustainable energy innovation. These photovoltaic devices harness the limitless energy of the sun. solar cell are starting to show promise in light of the global need to switch to cleaner, greener energy sources. By proving a sustainable substitute for traditional fossil fuels, these photovoltaic devices have the potential to revolutionize the energy production sector. The quick conversion of light energy into electrical energy by solar cells and known as photovoltaic effect which occurs as soon as a material absorbs light energy and produces current or voltage. Since the word photo implies light and volts refers to the quantity of energy utilization they are occasionally mentioned to as photovoltaic cells. Solar photovoltaic cells semiconductors which are special metals absorb photon from the sun. In a solar cell light energy moves quickly. When photons strike semiconductors, they create electricity rather than heat. Solar cells which convert solar light energy into electrical power are composed of semiconductors. Size of solar cell is really tiny.

They are frequently dark midnight blue in colour and have an octagonal shape. The electrical properties of a solar module are directly impacted by the amount of light it absorbs. These devices are categorized as photoelectric because light alters their electrical characteristics

such as resistance voltage and current often solar cells are combined to from bigger devices called solar panels or modules. One type of photovoltaic cell that can operate without artificial light or sunshine is a solar cell. In addition to producing energy solar cells are used as photo-detector also referred to as infrared detectors, to monitor light levels and detector near- visible or electromagnetic light. When light is absorbed, excitons or electron –hole pairs are created.

The maximum efficacy of solar cell (silicon solar cells) is usually 26.5%, [2] yet they are also very expensive. The Shockley-Queisser limit, or maximum efficiency, of a solar cell with a conventional and individual p-n junction layer was established in 1961 by William Shockley and Hans-Joachim. The efficiency of this limit has been measured at 33.7% [3]. The Shockley-Queisser limit only applies to single-layered solar cells.

Multi junction or multiple layer solar cells are supposed to have an efficiency of 84.8 percent, although their actual efficiency is closer to 28 percent [4]. It is believed that solar cells of the second and third generations will exceed this limit. The following phases explain how a solar cell functions: as photons from sunlight strike the panel surface, they are taken in by doped silicon and other semiconductor materials. Two distinct silicon layers are placed together to from a solar cell, which permits energy to pass through them in a certain direction. The inferior layer, also known as p-type or positive type silicon, is doped to have a very low electron count. The topmost layer, known as n- type or negative-type silicon, is doped to have a high electron. Electrons are then encouraged to leave their atomic or molecular orbitals. An electron may travel across the cell to reach the electrode following stimulations, or it may lose heat before returning to its original orbital. Electricity is created when the potentials are cancelled out by the current passing through the substance.

Silicon is usually used between two layers, one modified with boron and the other with phosphorous. The capacity of the substance to create chemical bonds is mostly what drives this process. These layers guide and accelerate the electron stream because of their varying electrical and chemical changes.

A collection of solar cells provides a useful amount of direct current (DC) electricity from solar radiation. With an inverter, electricity may be transformed into alternating current. Vast area, junctions called p-n junctions in silicon are typically used to make solar cells. An optically conducting film is placed on the side of solar cell that receives light to let light reach the active material and collect the generated charge carriers.

This is accomplished by using films that have high potential for electricity and transmittance, such conducting nanowires. Organic solar cells, dye-sensitized solar cells, perovskite solar cells, and quantum dot solar cells are additional battery kinds.

There are three main generation of solar cells-

1.1. Solar cell of the first generation

In the worldwide solar energy industry, crystalline silicon (c-Si), the most commonly used and practically proven technology, is the primary component of classic photovoltaic devices, which are referred to as the solar cell of first generation.[5]

The two primary categories are polycrystalline and monocrystalline silicon. Because they are made from a single uninterrupted crystalline unit, solar cells which is monocrystalline have consistent look and greater efficiency, usually around 18% and 22% [6].

Crystalline polymers silicon cells, on the other hand, are produced by fusing many silicon pieces together; this lowers production costs but results in somewhat lower efficiency, usually between 15% and 17%. Because of its high efficiency, dependability, and extended operating lifespan –which frequently exceeds 25 years under normal circumstances-These cells are widely used [7].

The solar cells of first generation have a number of drawbacks despite their benefits. Their expensive production expenses are one of their biggest disadvantages since costly to operate procedures, such the Czochralski technique for monocrystalline silicon, are needed to produce high –purity silicon wafers. Comparing this to more recent technology, the initial cost for installation is greater.

Their comparatively worse outcomes in dispersed or low light environment is another drawback; in the absence of direct sunshine, their efficiency sharply declines. In addition, compared to new thin or organic solar technologies, the production method has a greater environmental impact and wastes a lot of material during wafer slicing. These restrictions have prompted research into creating more affordable, adaptable, and ecologically friendly substitute for solar cells in later generations.

1.2 Solar cells of the Second Generation

Thin –film photovoltaic technologies were established in the second generation of solar cells in order to get around the stiff construction and expensive cost of conventional crystalline silicon cells. These solar cells are created by applying a thin layer or several layers of photoelectric materials, such as copper indium gallium selenide (CIGS), amorphous silicon (a-Si), or cadmium telluride (CdTe), on a range of substrates, including metal, glass, and plastic. Thin film solar cells are distinguished from first –generation cells by their compact, versatile design,

reduced production costs, and superior performance in high temperature and low light environments [8]. They may be used in curved surfaces, portable solar systems, and building – integrated photovoltaics (BIPV) because of these features. Second –generation solar cells can have distinct drawbacks, though. One key disadvantage is their reduced efficiency, which is much lower than that of crystalline silicon cells and usually ranges between 7%and 15% [9].

1.3 Solar Cells of the Third generation

In contrast to traditional solar cells, the latest generate of solar cells is a new class of developing photovoltaic technologies designed to achieve better efficiency and reduced production costs. These technologies -which include dye-sensitized solar cells (DSSCs), Perovskite solar cells, organic sunlight harvesting devices (OPVs), quantum dot cells, and multijunction solar cells- use cutting –edge material and designs in contrast to first and second-generation cells [10].
Perovskite photovoltaic cells have garnered a lot of interest among these because of their quick efficiency gains, which in a brief development time reached over 25% in lab environments [11]. The flexible, light-weight, and semi-transparent characteristics of third-generation solar cells make them appropriate for contemporary uses such a wearable technology, sophisticated windows, and handheld electronics.

In the quest for next-generation photovoltaic technology, perovskite solar cells- particularly those based on $FAPbI_3$-are a top candidate. By its unique crystal structure and tuneable optoelectronic properties, $FAPbI_3$ has the potential to achieve significant power conversion efficiencies at a relatively low cost.
This study aims to simplify the complications of $FAPbI_3$ solar cells, emphasizing design advancements and thorough evaluations to maximize their efficiency.

Performance Analysis
Researchers examine the solar cells fill factor, open circuit voltage, short circuit current and PCE. It also includes charge production/recombination/transport for improvement.

Opportunities
Higher Efficacy, Low Production cost and flexibility are the key drivers for more research in $FAPbI_3$ cells by using various methods.

2. Literature Review

Chapin et al. made the first silicon solar cell in 1954 at Bell Laboratory [12]. The earth receives $2.9X10^{15}$ KW of solar energy from the sun's electromagnetic radiation. To start with we deployed silicon wafers to produce electricity from sun light. Now these cells are built on the theory that semiconductors made of two different materials i.e. P-type and N-type which produce electron hole.

Solar cell combination i.e. solar panel used for commercial power production. However, some parts, like PV cells are very costly, and it will be challenging to integrate them into large scale businesses. These thin SI-based solar PV cells, which may attain up to 25% efficiency, are made of Organic, inorganic, or combinations of both that are used in third generation exciton Photovoltaic systems [13].

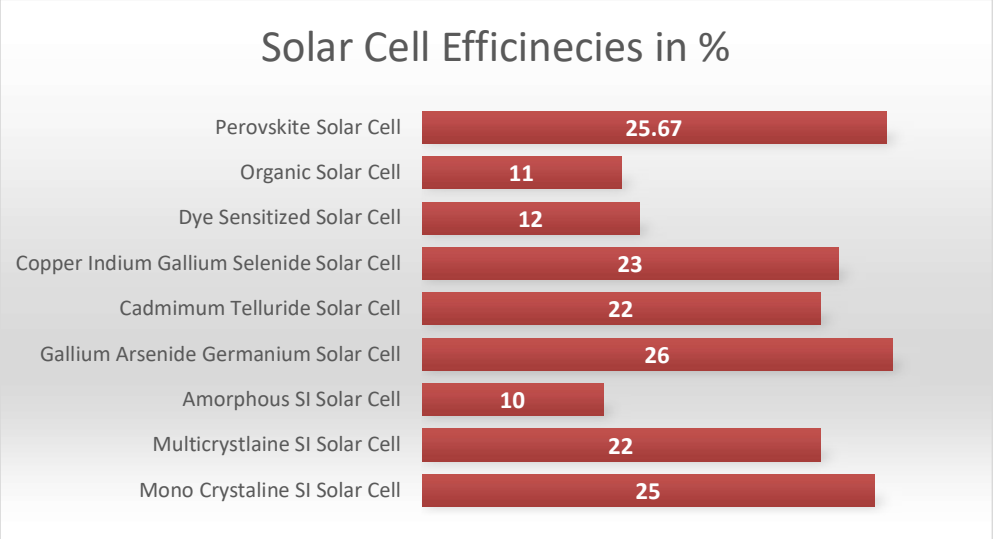

Fig-2 Various Solar Cell Efficiencies [14]

One of the most often used materials for solar cell production is silicon based on crystals. Over 90% of the worldwide market is covered by it. Pure silicon must be recovered by Reducing and purifying imperfect silicon dioxide in quartz to create a silicon chip. 99% pure molten silicon is produced at high temperature and processed through the floating zone, or "FTZ" [15]. A multiwire saw is used to cut the wafer, which is either 125 mm or 156 mm thick and made of either polycrystalline (lower cost, lesser efficiency) or single crystal (higher cost, greater efficiency).

Thin-film organic solar cells are the best suitable material for this use since they are easier to obtain and less expensive to manufacture than semiconductor materials. For wafers to absorb light, they must be extremely thin.

For organic photovoltaics to work, device physics, interfacial effects, and charge-separation and charge-transport mechanisms must all be considered. By employing materials with improved spectrum responsiveness, energy-level alignment, and transport characteristics, we will be able to design more stable and effective device topologies.

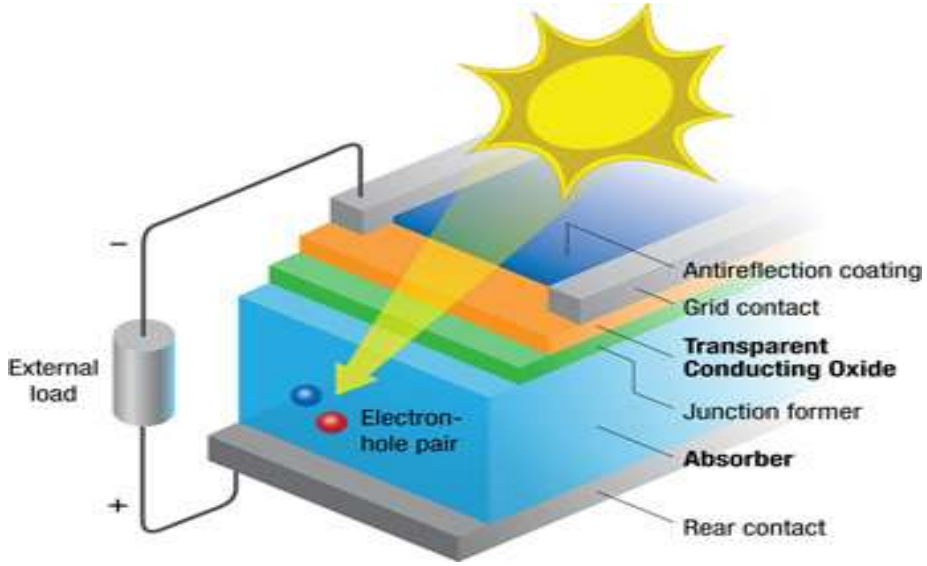

Fig-3 The Organic Photovoltaic Cell's (OPV) Working Principle [16]

100 nm thick material make up organic solar cell. The aim is to find substitute of the costly silicon used in photovoltaic cell and to employ less expensive production techniques are the driving forces behind the usage of organic dyes. Furthermore, because organic solar cells can be produced on plastic foil, they are best for transport & are supple in nature [17].

Organic solar cells consist of the following fundamental layers: the first electrode, hole transmission layer, photoactive section, electron transmission layer, and second electrode.
In a typical solar, light is collected, the electrons and holes it creates are separated and energy is then sent to the contacts. Direct generation of free charge carriers differentiate between

inorganic & organic solar cell. When light captivated by organic materials, excitons are produced; these particles typically have a binding energy of 0.3 to 0.5eV [18].

Exciton is often separated at the line amid two diverse organic layers (hetrojunction) since an organic solar does not have the electric field ($>10^6$ Vcm^{-1}) required to overcome this binding energy. To effectively separate the excitons while preventing any energy loss during the operation, these two-materials energy alignment has to be changed.

Conventional silicon-based solar cells need multistep manufacture, expansion high temperature and vacuum equipment. Perovskite solar cells as opposed to traditional third generation photovoltaics may also represent a novel idea and design. Furthermore in 1990, Michal Gratzel and Brian O'Regan demonstrated dye-sensitized solar cells (DSSC) remarkable efficiency [19]. A metal oxide anode that can be regenerated with a liquid iodide electrolyte or a solid-state hole extraction layer typically a tiny organic molecule is used in dye sensitized solar cell to create an organic semiconductor. In essence, these are photoelectrochemical systems which improve the way the dye and light anode interact.

The first PSC prototype was developed in 2009 using a liquid DSSC structure with a perovskite absorber instead of a conventional dye. Perovskite is the term used to describe the crystalline structure of absorber material ABX_3 [20]. This material is conceptually a hybrid organolead halide compound that was deposited utilizing a conventional solution process approach after being produced through a comparatively simple synthesis.

Previous studies have found super structured solar cells based on organometallic halide perovskite with promising photovoltaic efficiency (T. Miyasaka et al. The surface of super structured materials like TiO_2 or Al_2O_3 is coated with a thin layer of PbI_3 (organo-lead iodide) perovskite material that is well-oriented [21]. It is act as a light harvester and carrier conductor. These devices use a straightforward spin coating technique with a sub micrometre crystal structure. To boost efficiency in the case of perovskite materials, researchers are also concentrating on the excited state and charge transfer mechanism. Excellent power conversion efficiency PCE is a feature of all solid-state mesoscopic solar cell and they hold tremendous promise for practical uses. F.Meillaud et al. previously claimed that amorphous silicon, copper indium gallium selenide (CIGS), or CdTe thin film solar cells may be manufactured at a very low cost as a substitute for crystalline silicon cells [22]. Better mechanical qualities and a wider range of applications are offered by perovskite solar cells, albeit at the expense of decreased efficiency. Perovskite, organic, dye-sensitized, tandem, and other "third generation" solar cells report for a wide range of concepts, from low-cost, low-efficiency systems (organic solar cells, perovskite organic hybrid solar cells) to high-cost, high-efficiency systems (III–V

multijunction), with a variety of applications ranging from building amalgamation to space applications.

Compared to silicon-based sun cells, thin-film solar cells utilize less material per surface, do not require silver electric connections, and do not require costly purification procedures. As a result, despite being manufactured in far smaller quantities, thin-film devices perform comparably to silicon-based solar cells in terms of embedded energy, energy payback time and cost [23].

Currently, research is also using a variety of quantum dot materials to improve the power conversion (PCE) efficiency of solar cells by integrating them into the heterojunction structure of the cells. Mengqin King et al.'s consideration of nontoxic $(CH_3NH_3)_3$ Bi_2I_9 perovskite solar cells free of holes conductors with an alternative architectural design and a solution processable approach may encourage further study and practical application of lead-free organic-inorganic hybrid perovskite solar cells. The two-step soaking process was used for the first time to produce M.B.I. films. M.B.I. films produced on a planar and mesoporous TiO_2 layer, respectively, and the 1s technique are inferior to the 2s technique in this investigation [24].

Compared to conventional TiO_2, SnO_2 has superior optical and electric characteristics, stability, and band alignment to perovskite, making it a theoretically more plausible choice for extremely effective PSCs. Due to its exceptional optical transparency in the visible spectrum, photovoltaic cells and solar energy conversion devices are eager to use it for commercial purposes, resulting in inadequate electrical and interfacial contact, as well as an energy level that is out of alignment with nearby perovskite. Furthermore, LTP SnO_2 has shown to be a great ETL material for productive PSCs and is inexpensive and simple to operate SnO_2's relatively high band gap enables less absorption of UV radiation and enhanced device stability. Additionally, the SnO_2's reduced hygroscopicity and resilience to acidity add to the PSC device's endurance [25].

X. Zhang et al. claim that the photovoltaic efficiency of the perovskite solar cell based on the SnO_2 electron transport layer has been remarkably high. But there are a lot of problems with the commercial SnO_2 ETLs. Due to its accumulating property, the SnO_2 forerunner is deformed in shape and contains many interface defects. Additionally, the open circuit voltage (V_{oc}) would be constrained by the distinct energy levels of SnO_2 and perovskite. Also, only a few studies have developed SnO_2-based ETLs that promote PbI_2 crystal formation, which is necessary to produce superior perovskite films utilizing the 2-step method [26].

Here, we effectively addressed the previously described issues by putting forward a novel dual SnO_2 architecture that combined sol-gel solution with atomic layer deposition.

Because of its unique conformal impact, ALD-SnO_2 can efficiently modify the FTO substrate's roughness, enhance the quality of ETL, and promote the development of the PbI_2 crystal state to increase the crystallinity of the perovskite layer. The intrinsic field of a bilayer SnO_2 can also help to inhibit electron accumulation at the ETL/perovskite interface, which raises the fill factor and Voc. In a N_2 atmosphere with 20% humidity, the efficiency of PSCs using ionic liquid solvent increases from 22.09% to 23.86%, maintaining the initial 85% efficiency for 1300 hours [27].

2. Description of Broad Area

A tiny portion of the energy released by the sun falls to the earth. We refer to these as photons. Energy is released when a photon strikes an atom. Solar energy is the planet's most abundant and pure energy source. A solar cell and the photovoltaic effect, which produces current or voltage in a substance by absorbing light energy, are used to directly convert light energy into electrical energy.

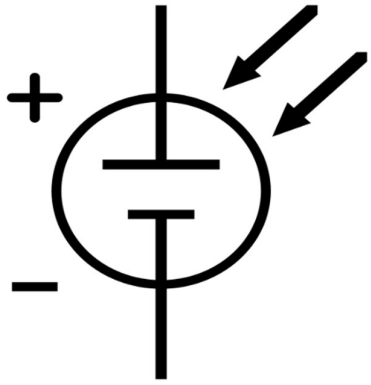

Fig-4 Symbol of solar cells

They are called as photovoltaic cells because the letters photo and volts stand for light and electricity, respectively. When Photons fall on solar cell they generate electricity & not heat. Semiconductors are required to made any kind of solar cell. They are midnight blue visibly. The amount of sun light fall on the cell can increase or decrease the amount of production and its properties i.e. current, voltage and resistance etc. It is applicable for sun light or artificial light. Solar cells can also work as a photo detector which can be used to know the amount of electromagnetic energy.

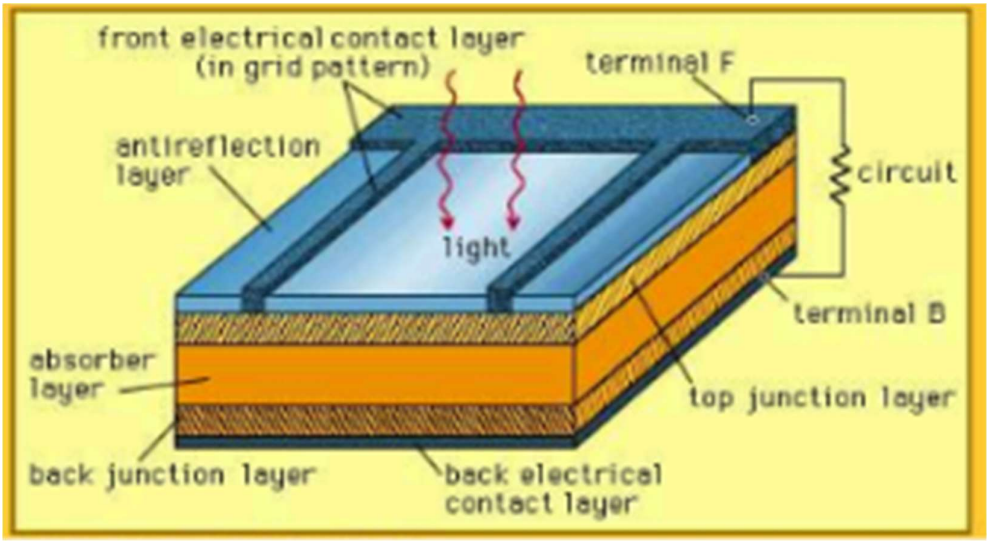

Fig-5 Principal of Conversion light into electricity [28]

The three characteristics that are necessary for a photovoltaic cell (PV cell) to function are: Electron-hole pairs called excitons are created when light is absorbed. The opposite types of charge carriers are then determined. The distinct charge carriers are then transferred to an external circuit.

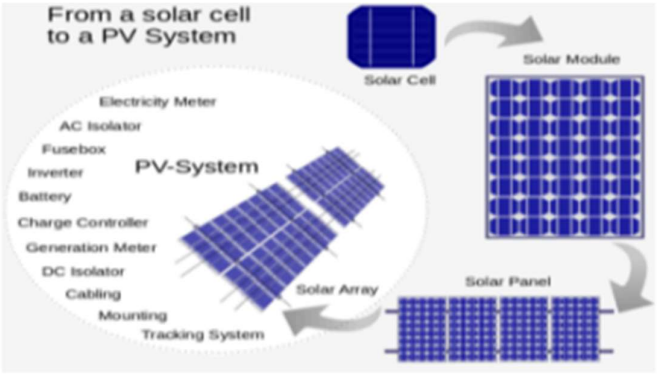

Figure-6 Solar Cell to PV System [29]

The maximum efficiency of solar cells (silicon solar cells) is usually 26.5%, yet they are also very expensive. The Shockley-Queisser limit, or maximum efficiency, of a solar cell with a conventional and individual p-n junction layer was established in 1961 by William Shockley and Hans-Joachim. The efficiency of this limit has been measured at 33.7%. However, only single -layered solar cells are vulnerable because of the Shockley - Queisser limit. Even if

the productivity of multiplex junction or multiple layer solar cells is closer to 28%, it is expected to achieve 84.8% [30]. Solar cell of 2nd and 3rd Peers are expected to exceed this limit.

4. Objectives of the Study

Our aim is to use SCAPS (Solar Cell Capacitance Simulator)-1D modeling software to examine the characteristics of a thin film $FAPbI_3$ perovskite solar cell for below issues by varying thickness & doping concentration.

1. To increase the $FAPbI_3$ Solar Cell's Power Conversion Efficiency (PCE) by adding a Layer of SnO_2 as an Electron Transport Layer.
2. To increase the $FAPbI_3$ Solar Cell's Power Conversion Efficiency (PCE) by adding a NiO layer as a Hole Transport Layer.
3. Using a Bilayer Electron Transport Layer and a Bilayer Hole Transport Layer to Boost Perovskite Solar Cell Stability and Power Conversion Efficiency.

5. Methodology

In order to improve the PCE, the solar cell's structure will first be simulated using SCAPS software before being tested in a lab. Perovskite solar cells have collected a lot of interest recently due to its exceptional efficiency and promise for lower production costs. We will use SCAPS to digitally simulate the different layers and compositions in order to improve the stability and efficiency of the solar cell.

SCAPS is a well-known software application for simulating many types of solar cells, including perovskite solar cells. There are the brief features of SCAPS which provide the information and in-depth description of each layer of solar cell as below.

- Thickness (nm)
- Bandgap (eV)

Electron affinity (eV)

- Permittivity (relative)
- Effective density of states (conduction & valence bands)
- Doping concentration (cm^{-3})
- Mobility of electrons and holes ($cm^2/V \cdot s$)
- Interfaces: Set up interface properties between layers

- Interface recombination velocities
- Defect states at interfaces
- Contacts: Define front and back contacts
- Work function (eV)
- Type (Ohmic or Schottky)
- Reflection and absorption properties

5.1 Operating Conditions-

5.1.1 Illumination Settings: AM1.5G spectrum (standard solar illumination) or custom spectrum Light intensity (e.g., 1000 W/m²), Monochromatic light simulations.

5.1.2. Temperature: Simulation temperature (typically 300 K for standard testing)

5.1.3 Bias Voltage Range: Set voltage sweep range for J-V characteristics (e.g., -1 V to +1 V)

5.2. Defects and Recombination Parameters

5.2.1 Bulk Defects: It defines defect energy levels, concentrations, and capture cross-sections. Surface and interface defects, Include possible recombination centers at surfaces/interfaces.

5.2.2 Calculation Outputs

- J-V curves
- Quantum efficiency (QE) spectra
- Capacitance-voltage (C-V) characteristics
- Energy band diagrams

5.2.3 Running and Analyzing Simulations

- Run simulations and analyze outputs
- J-V Curves: Extract Voc, Jsc, FF and efficiency
- QE Analysis: Determine spectral response and losses, Energy Band Diagrams, Study band alignments and potential barriers

6. Expected outcome of Research

After optimization of parameters, the PCE of the device will be improved. However, these optimized parameters will also be used in fabrication of solar cell in laboratory. The results will be published in peer review Journals.

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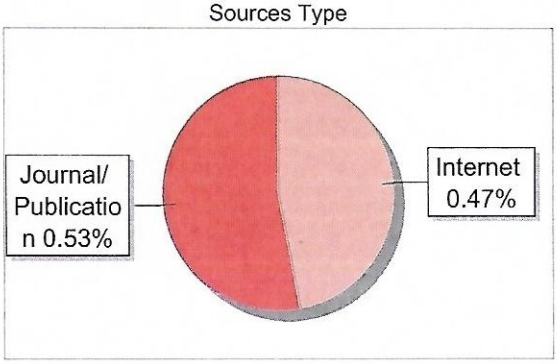

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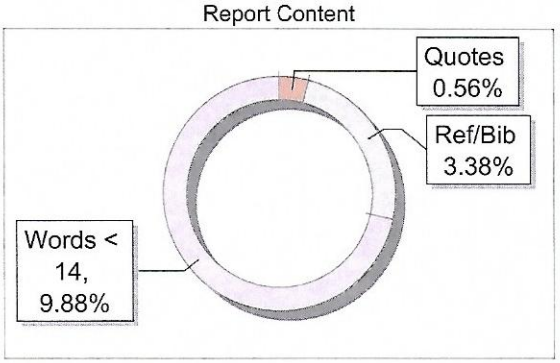

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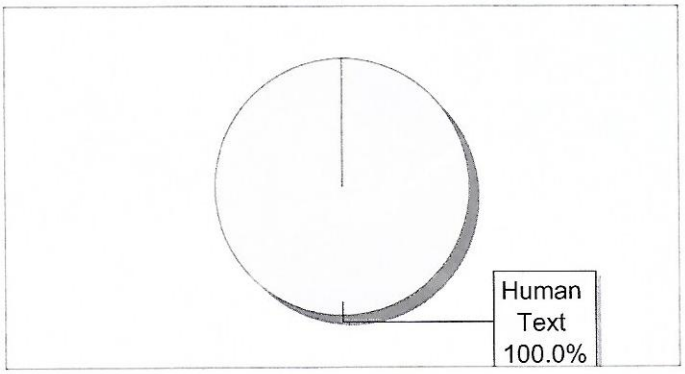

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